

**MS22 O1**

**Single crystal diffraction at extreme pressures** Michael Hanfland<sup>a</sup>, H. Müller<sup>a</sup>, K. Syassen<sup>b</sup>, <sup>a</sup>ESRF, Grenoble, France, <sup>b</sup>MPI für FKF, Stuttgart, Germany  
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**Keywords:** high pressure, single crystal, diffraction

Technical advances have considerably added to the utility of single crystal studies at high pressures. New ways of supporting diamond anvils, like Boehler Almax anvils [1], have significantly increased the volume of accessible reciprocal space. Use of He as pressure transmitting medium extends substantially the practicable pressure range. Here we will present two examples to illustrate the recent progress.

In the first example single crystals of  $\alpha$ -ET<sub>2</sub>I<sub>3</sub> [2] were loaded in LeToullec type membrane driven diamond anvil cells, modified for Boehler-Almax anvils with He as pressure transmitting medium. Datasets with 2° rotation images were taken at various pressures to 23 GPa with a Mar image plate scanner on the ID9A beamline of the ESRF. Total rotation range was 60°. The datasets were measured at photon energy of ~30keV and integrated with XDS [3]. The  $\alpha$ -phase of ET<sub>2</sub>I<sub>3</sub> is stable to 13 GPa. At 13 GPa it undergoes a structural phase transition. The high pressure phase, which remains single crystalline, can be indexed with a triclinic unit cell with twice the volume than that of  $\alpha$ -ET<sub>2</sub>I<sub>3</sub>. The transition is reversible.

The second example deals with the guest host structure observed in Na at pressures above 125 GPa [4].

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[2] Work done in collaboration with H. Müller  
[3] W. Kabsch, *J. Appl. Cryst.*, 1993, 26, 795  
[4] Work done in collaboration with K. Syassen

**MS22 O2**

**Nanocage materials under high pressure** A. San-Miguel, R. Poloni, N. Rey, P. Toulemonde, S. Le Floch, D. Machon and V. Pischedda *LPMCN, University of Lyon and CNRS, Lyon, France.*  
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**Keywords:** high pressure, fullerene, clathrate

The study of nanomaterials under extreme conditions constitutes an expanding domain relevant for fundamental science as well as for applications [1]. Nanocage materials are particularly interesting in this context. In fact, their open structures allow for complex host-guest interaction which can be modulated by pressure. On the other side the combination of pressure and temperature can allow for the formation of new assemblages giving rise to novel nanomaterials.

Recent results on two important cases of nanocage intercalated materials will be here discussed: group 14 clathrates and intercalated fullerenes. They are well differentiated systems due to the type of interactions between the nanocages, the size of the cages and the preferred intercalation modes [1]. We have recently reviewed the high pressure properties of group 14 clathrates [2]. The high pressure behavior of silicon

clathrates is dominated by the extended stability of the structure due to nanointercalation and by the presence of an homothetic isostructural volume collapse [3] which nature is under debate and is giving rise to an important number of studies and publications. Our discussion will be centered on these aspects.

In the case of intercalated fullerenes, recent results on the construction of the first pressure-temperature phase diagram of alkali intercalated C<sub>60</sub> fullerenes will be presented.

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[2] San-Miguel A. And Toulemonde P., *High Pressure Research*. 2005, 25, 159.  
[3] A. San-Miguel, A. Merlen, P. Toulemonde, T. Kume, S. Le Floch, A. Aouizerat, S. Pascarelli, G. Aquilanti, O. Mathon, T. Le Bihan, J.P. Itié and S. Yamanaka, *Europhysics Lett.* 2005, 69, 556.

**MS22 O3**

**Pressure-induced phase transitions in hydrides** Igor Goncharenko<sup>a</sup>, Olga Makarova<sup>b</sup>, Michael Hanfland<sup>c</sup>, <sup>a</sup>Laboratoire Léon Brillouin CEA-CNRS, 91191 Gif-sur-Yvette, France. <sup>b</sup>Russian Research Center “Kurchatov Institute”, 123182 Moscow, Russia. <sup>c</sup>European Synchrotron Radiation Facility, BP 220, 38043 Grenoble, France. E-mail: [Igor.Goncharenko@cea.fr](mailto:Igor.Goncharenko@cea.fr)

**Keywords:** pressure, diffraction, phase transitions

We report pressure-induced magnetic and structural transitions in hydrides studied by a combination of X-ray and neutron probes in 100 GPa pressure range.

Hydrides of metals exhibit very unusual coupling of structural, magnetic and transport properties. In our previous studies we had reported a pressure induced magnetic collapse in the cubic Laves hydrides formed by rare-earth and transition metals [1,2]. Our recent studies, extended to new type hexagonal hydrides, evidenced new peculiar phenomena. Under high pressure, we observed both “magnetic amorphization” and “magnetic crystallization”. The complexity of magnetic phenomena comes from a competition of different interactions and peculiar crystal structure of these compounds.

Whereas the hydrides of rare-earth or transition metals (right-down part of the periodical table) are typically metals, the hydrides formed by elements from the left-upper corner of the periodic table are insulators bonded by ionic or covalent bonds. Under high pressure, these hydrides might form “hydrogen dominant” phases recently suggested by theory [3]. We report new pressure-induced crystal structures and important changes in interatomic bonding in these hydrides.

Possibility to carry out X-ray and neutron measurements on the same sample in the same thermodynamical conditions of pressure and temperature provides new opportunities for high-pressure studies [4], especially for studies of magneto-structural coupling or structural transitions involving light elements. We describe new pressure techniques and discuss further prospects for single-crystal and powder diffraction under very high pressures.

- [1] I Goncharenko, P. Cadavez-Peres, I. Mirebeau, O. Makarova, *Europhys. Lett.*, 2001, 54, 807.